Detection of $HC_{11}N$ in the Cold Dust Cloud TMC-1

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ABSTRACT

Two consecutive rotational transitions of the long cyanopolyyne $HC_{11}N$, $J = 39 \rightarrow 38$ and $38 \rightarrow 37$, have been detected in the cold dust cloud TMC-1 at the frequencies expected from recent laboratory measurements by Travers et al. (1996), and at about the expected intensities. The astronomical lines have a mean radial velocity of 5.8(1) km s^{-1}, in good agreement with the shorter cyanopolyynes HC_7N and HC_9N observed in this very sharp-line source [5.82(5) and 5.83(5) km s^{-1}, respectively]. The column density of $HC_{11}N$ is calculated to be 2.8×10^{11} cm^{-2}. The abundance of the cyanopolyynes decreases smoothly with length to $HC_{11}N$, the decrement from one to the next being about 6 for the longer carbon chains.

Subject headings: ISM: abundances — ISM: molecules — line: identification — molecular data — molecular processes — radio lines: ISM

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1. Introduction

Several weak radio lines in the circumstellar shell of IRC+10216 (Bell et al. 1982) and the dust cloud TMC-1 (Bell & Matthews 1985) were originally attributed to the long carbon-chain molecule $HC_{11}N$ (cyano-deca-penta-yne), but a sensitive spectral survey of IRC+10216 between 22.3 and 24.1 GHz (Bell unpublished) showed no evidence for this molecule at other frequencies predicted from the earlier assignment. This anomaly has now been explained with the laboratory detection of $HC_{11}N$ by means of a Fourier transform molecular-beam spectrometer which showed that the earlier assignment was incorrect (Travers et al. 1996). Although the deep IRC+10216 spectral survey also showed no evidence for spectral lines at the $HC_{11}N$ laboratory frequencies (Bell, Feldman, & Avery 1992; Bell et al. 1992), the laboratory data have permitted a very deep astronomical search for this molecule in the narrow-line source TMC-1, and this has now been done with the new, very sensitive, dual-polarization GBT receiver in operation on the NRAO[5] 140-foot (43 m) telescope. We report here the detection in TMC-1 of two transitions of $HC_{11}N$ near 13 GHz, close to the expected line intensity peak for a source at 10 K.

2. Observations and Results

The observations were done in two sessions with the 140-foot telescope, both during excellent weather. In 1996 December the $J = 39 \rightarrow 38$ line at 13186 MHz was observed for a total of 35 hours and in 1997 January the $38 \rightarrow 37$ line at 12848 MHz was observed for a total of 36 hours. The observations during the second session were undertaken remotely from Ottawa by means of the 140-foot DISPLAY software.

Telescope pointing difficulties encountered in both sessions sometimes required pointing checks every 30 minutes. For this reason, during most of each session a nearby transition of HC_9N was observed simultaneously in the second correlator bank, which is available for independent observations even when the dual-polarization receiver is used (provided that the autocorrelator is set in the 4-bank mode). In both sessions, on starting observations each day the $J = 5 \rightarrow 4$ transition of HC_5N at 13313 MHz and the $12 \rightarrow 11$ transition of HC_7N at 13536 MHz were also measured. To calculate accurate line intensities we also observed HC_5N and HC_7N near the meridian, so telescope gain changes could be estimated and corrections applied during data reduction.

For the $HC_{11}N$ observations, three different local-oscillator (LO) frequencies were used over the two sessions so that features that moved with the LO frequency could be recognized. With the narrow line widths in TMC-1 (0.5 km s^{-1}, or 20 kHz at 13 GHz), spectral features of terrestrial origin are smeared over several line widths during the 4-5 day observing sessions. Sharp features that are present in each night's average, or in both the first and last halves of the data, must then be either source-related or an artifact introduced by the correlator. Since the $HC_{11}N$ spectra were in banks 2 and 4 in December and banks 1 and 3 in January, U lines that occur in different channels in the two sessions might still be correlator related. Because of the change of banks between the two sessions, however, the appearance of the $HC_{11}N$ line at the expected position in both sessions is highly unlikely to be of instrumental origin. Although spectral baseline ripple is not usually a problem when frequency switching with small offsets (± 29 kHz) on narrow-line sources, the normal $\pm\lambda/8$ focus modulation that removes ripple produced by residual standing waves between the primary and secondary reflectors was also employed as a precaution.

In December the observed frequencies were near the center of the receiver passband and sys-

[5]The National Radio Astronomy Observatory (NRAO) is operated by Associated Universities Inc., under agreement with the National Science Foundation.

tem temperature was about 28 K; in January they were closer to the edge of the band and the system temperature was about 33 K. The telescope beamwidth (FWHM) was 2.′4 and the beam efficiency was 0.54 (C. Brockway, personal communication 1992). The observing technique used was small-offset frequency switching; the frequency-switched images were later removed as described previously (Bell, Avery, & Watson 1993; Bell 1996; Bell 1997). The autocorrelator was configured with 4 banks (2 for each polarization), each with 256 channels. The frequency offset used for HC_9N and $HC_{11}N$ was ± 6 channels. An offset of ± 16 channels was used for HC_5N and HC_7N because of the hyperfine splitting of the HC_5N transition. Taking both polarizations into account, the effective on-source integration time for $HC_{11}N$ was about 70 h in each session.

Spectra containing the two observed transitions of $HC_{11}N$, and the $J = 23 \rightarrow 22$ transition of HC_9N observed simultaneously with the $39 \rightarrow 38$ transition of $HC_{11}N$, are presented in Figure 1 plotted on a common velocity scale. All three spectra have been processed in an identical fashion, which included overlapping, removing the reference images, and Hanning smoothing. The line parameters are presented in Table 1. The rest frequency obtained from laboratory work is included in column 2, the measured LSR velocity is in column 3, the brightness temperature is in column 4, and the measured line width (FWHM) is in column 5. As can be seen from column 3, the velocities measured for HC_7N and HC_9N are close to the value of 5.85 km s^{-1} expected for this source (Kroto et al. 1978; Tölle et al. 1981). Although the velocities of the $HC_{11}N$ lines have larger uncertainties because of the poorer signal to noise, the mean value obtained from the two transitions (5.84 km s^{-1}) is in excellent agreement with the values found for the shorter cyanopolynes. The lines identified as $HC_{11}N$ also have widths normal for TMC-1.

It should be noted that in some cases the observing frequency used differed slightly from the rest frequency listed in column 1 of Table 1. For HC_5N the observing frequency used was 13313.338 MHz. More importantly, for the HC_9N $J = 22 \rightarrow 21$ and $23 \rightarrow 22$ lines the observing frequencies were 12782.766 MHz and 13363.790 MHz, respectively, and the differences between these and the rest frequencies in Table 1 were taken into account in determining velocities. For the $J = 38 \rightarrow 37$ line of $HC_{11}N$, the value obtained from the laboratory constants, 12848.731 MHz, was used both as an observing frequency and in determining the velocity listed in Table 1.

Three U lines are apparently present in the deep $HC_{11}N$ spectra in Figure 1. For the reason mentioned earlier we are unable to rule out completely the possibility that these are spurious features introduced by the correlator. If this is the case, however, they are seen only at very low levels. From the two $HC_{11}N$ spectra, the line density at this level ($\sim$ 2mK) is estimated to be ~ 2 lines per MHz. It is easily shown that with this line density the chance of detecting a U line within one channel (4.88 kHz) of the expected $HC_{11}N$ position is about 1%, and the probability of this happening for two transitions is thus very small: $\sim 10^{-4}$. The probability of finding lines at the right frequencies with the right intensities and widths is clearly even less, so the identification of $HC_{11}N$ in space now seems quite secure.

Spectra obtained for HC_5N and HC_7N (after 4 and 20 minutes of integration, respectively) are shown in Figure 2 after overlapping. In these cases overlapping has been done but their frequency-switched images have not been removed. To determine the integrated line intensity of HC_5N, the area under the three quadrupole hyperfine components was summed. To obtain the final single-component peak equivalent value, the total area was then divided by 0.4 km s^{-1} which was assumed to be the velocity width (FWHM) of the source (Broten et al. 1978).

Column density estimates were made for all four observed cyanopolyyne molecules on the as-

sumption that (i) all lines are optically thin, (ii) all lines originate from a source of size 6.′0 by 1.′3 (Churchwell et al. 1978; Olano et al. 1988), and (iii) the excitation temperatures are identical (i.e., there is a single rotational temperature). Calculations were carried out for rotational temperatures (T_{rot}) of 6, 8, 10, and 12 K, following the analysis of Avery et al. (1992). Although it might be thought that molecules with the very large dipole moments ($>$ 4 D) of the present cyanopolyynes would cool quickly and have rotational excitation temperatures lower than the kinetic temperature of the gas, this is not expected to be the case for the low-lying transitions observed here. Since the Einstein A coefficients are proportional to $\nu^3\mu^2$, the radiative cooling rates remain small even for transitions as high as $J = 40$, and the excitation temperatures are therefore expected to be close to the kinetic temperature. If so, the excitation temperature of $\sim$ 11.5 K recently determined for HC_9N in TMC-1 by Bell et al. (1997) is probably a good measure of the kinetic temperature of the gas in this source (c.f. Dickman 1975; Avery 1980).

The dipole moments used in the excitation analyses are listed in Table 2 along with the column densities calculated for T_{rot} = 10 K. The dipole moments quoted by Snyder et al. (1986) for HC_7N, HC_9N and $HC_{11}N$, which were based on crude ab-initio self-consistent field (SCF) calculations and modified by making empirical adjustments and extrapolation, are probably too low by as much as 0.5 Debye. Recently, large-scale coupled cluster [CCSD(T)] calculations have been carried out for HC_7N, HC_9N, and $HC_{11}N$ by P. Botschwina (personal communication 1997). He finds $\mu_0(HC_7N) = 4.82(5)$ D, $\mu_0(HC_9N)$=5.20(5) D, and $\mu_0(HC_{11}N)$=5.47(5) D. These values are estimated to be accurate to within a few percent, even though HC_7N to $HC_{11}N$ fall in the strongly non-linear part of the dipole-moment curve with respect to carbon-chain length. The column density found here for HC_9N, 1.9×10^{12} cm^{-2}, is slightly lower than the value 3.2×10^{12} cm^{-2} reported by Broten et al. (1978), although the dipole moment of this molecule turns out to be slightly lower ($\sim$ 7%) than their estimate of 5.6 D. This is largely due to the higher antenna temperature that Broten et al. reported for the $25 \rightarrow 24$ transition at 14535 MHz, which is almost 50% higher than we would now predict.

The calculated column densities are plotted for all four molecules in Figure 3 (upper), for excitation temperatures of 6, 8, 10, and 12 K. As the Figure shows, the abundance of $HC_{11}N$ does not vary significantly for excitation temperatures between 8 and 12 K. Figure 3 (upper) also shows how the abundance changes with the length of the cyanopolyyne chain, and how the decrements in abundance steepen as the excitation temperature increases. This can be seen more clearly in Figure 3 (lower) where, for T_{rot} = 10 K, the decrements are slightly larger than the value of $\sim$ 4 found previously by Broten et al. (1978) — they approach the earlier value, however, when lower excitation temperatures are assumed.

The present detection of $HC_{11}N$, a molecule with molecular weight (147 amu) nearly twice that of glycine, demonstrates that detectable quantities of fairly large organic molecules can form in astronomical sources under conditions markedly different from those on Earth. However, if the column densities of these carbon chains continue to drop at the rate observed for the longest cyanopolyynes, the most intense lines of the next longer cyanopolyyne, $HC_{13}N$, are unlikely to be stronger than $\sim$ 1 mK. If so, detection of this molecule in TMC-1 is likely to require the smaller, more efficient beam of the 100 m Green Bank Telescope now under construction by NRAO.

We wish to thank George Liptak and the 140-foot telescope operators for their assistance, especially during the remote observing session. We thank Ron Maddalena for providing the very useful DISPLAY software package required to carry out the remote observations. One of us (MBB) also thanks Pierre Brault for his assistance in

writing the LINECLEAN software and Jim Watson for helpful information and discussions on molecular physics.

TABLE 1
LINE PARAMETERS IN TMC-1[a]

Molecule (Transition)	Rest Frequency (MHz)	$v_{\rm LSR}$ (km s^{-1})	$T_{\rm B}$[b] (mK)	FWHM (km s^{-1})
HC_5N ($J = 5 \rightarrow 4$)	13313.3[c]	——	1770(43)	0.4[d]
HC_7N ($12 \rightarrow 11$)	13535.991[e]	5.82(5)	475(13)	0.53(2)
HC_9N ($22 \rightarrow 21$)	12782.769[f]	5.84(5)[g]	81.3(15)	0.40(1)
HC_9N ($23 \rightarrow 22$)	13363.800[f]	5.84(5)[g]	82.2(22)	0.38(1)
$HC_{11}N$ ($38 \rightarrow 37$)	12848.728[h]	5.73(10)	9.4(17)	0.36(10)
$HC_{11}N$ ($39 \rightarrow 38$)	13186.853[h]	5.96(10)	5.4(7)	0.56(10)
U(13186.46)		5.85	4.8(7)	0.26(10)
U(13186.98)		5.85	6.3(11)	0.26(7)
U(12848.48)		5.85	7.4(20)	0.26(6)

[a] $\alpha_{1950} = 04^{\rm h}\ 38^{\rm m}\ 39.3^{\rm s}$, $\delta_{1950} = 25^\circ\ 35'\ 36''$

[b] $T_{\rm B} = (T_{\rm A}^*)/\eta_B$ (uncorrected for beam dilution)

[c] From Alexander et al. 1976

[d] Assumed value

[e] From Kroto et al. 1978

[f] From Travers 1996 (unpublished)

[g] After adjustment for the observing frequency used (see text)

[h] From Travers et al. 1996

TABLE 2

CYANOPOLYYNE COLUMN DENSITIES IN TMC-1 FOR $T_{\rm rot} = 10$ K

Molecule	Dipole Moment (μ_0) (Debye)	N_L (10^{11} cm^{-2})[a] (cm^{-2})	Abundance Decrement
HC_5N	4.33[b]	330	
HC_7N	4.82[c]	110	3.0
HC_9N	5.20[c]	19	5.8
$HC_{11}N$	5.47[c]	2.8	6.8

[a]Adopting a beam-dilution factor of $(1.'3/2.'4) = 0.54$ (because the source is extended in one dimension; see Broten et al. 1978)

[b]From Alexander et al. 1976

[c]From P. Botschwina 1997 (personal communication)

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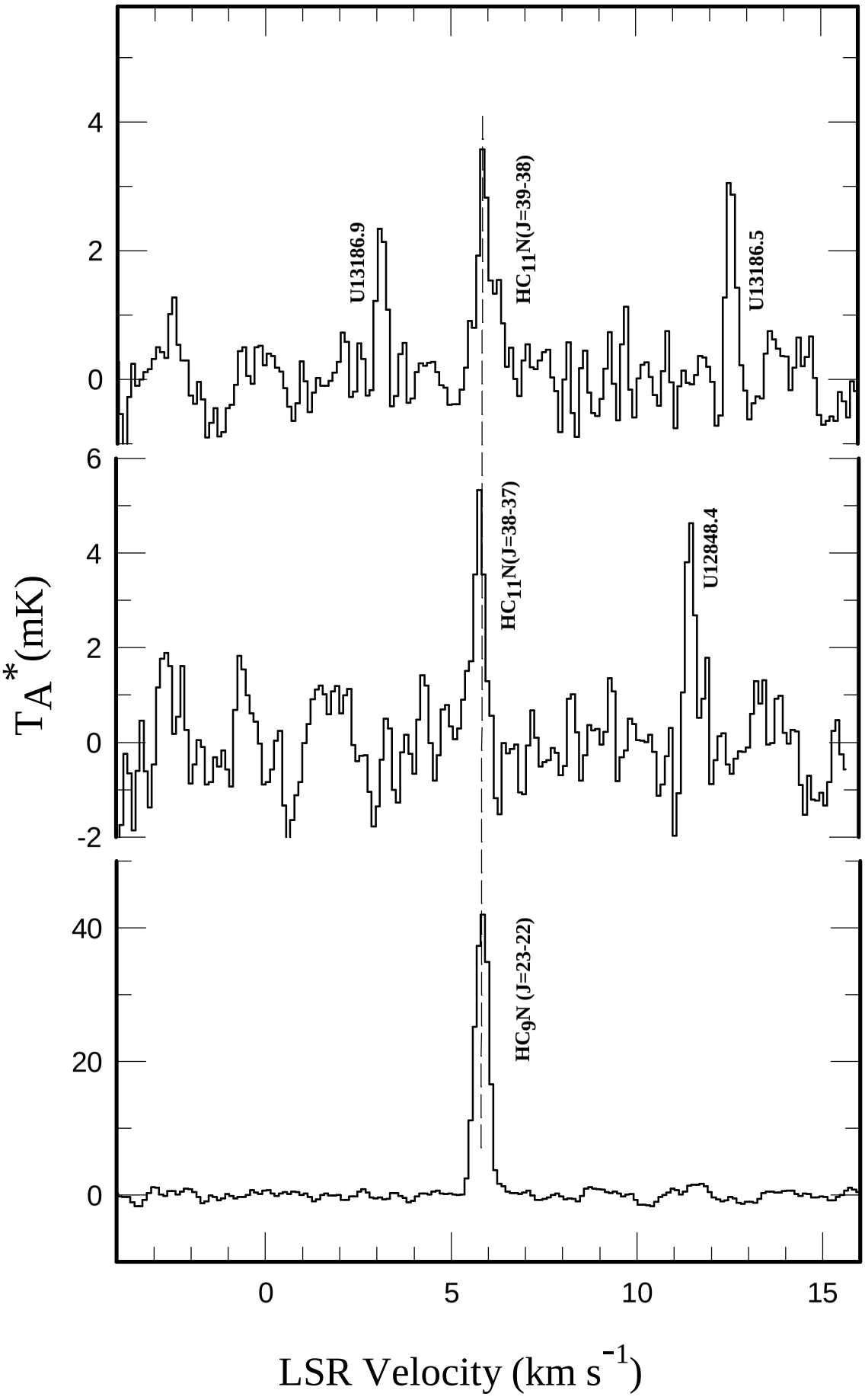
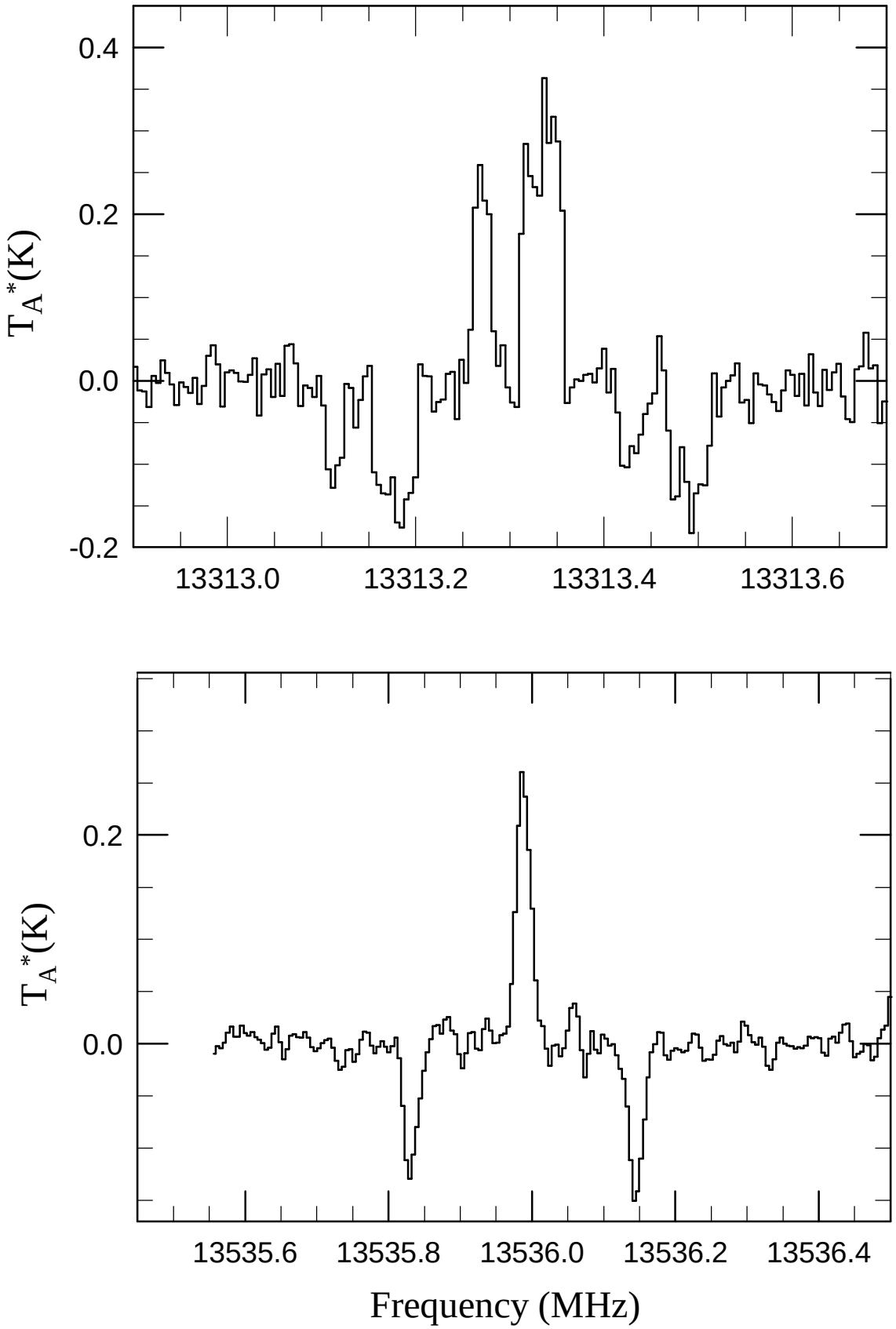
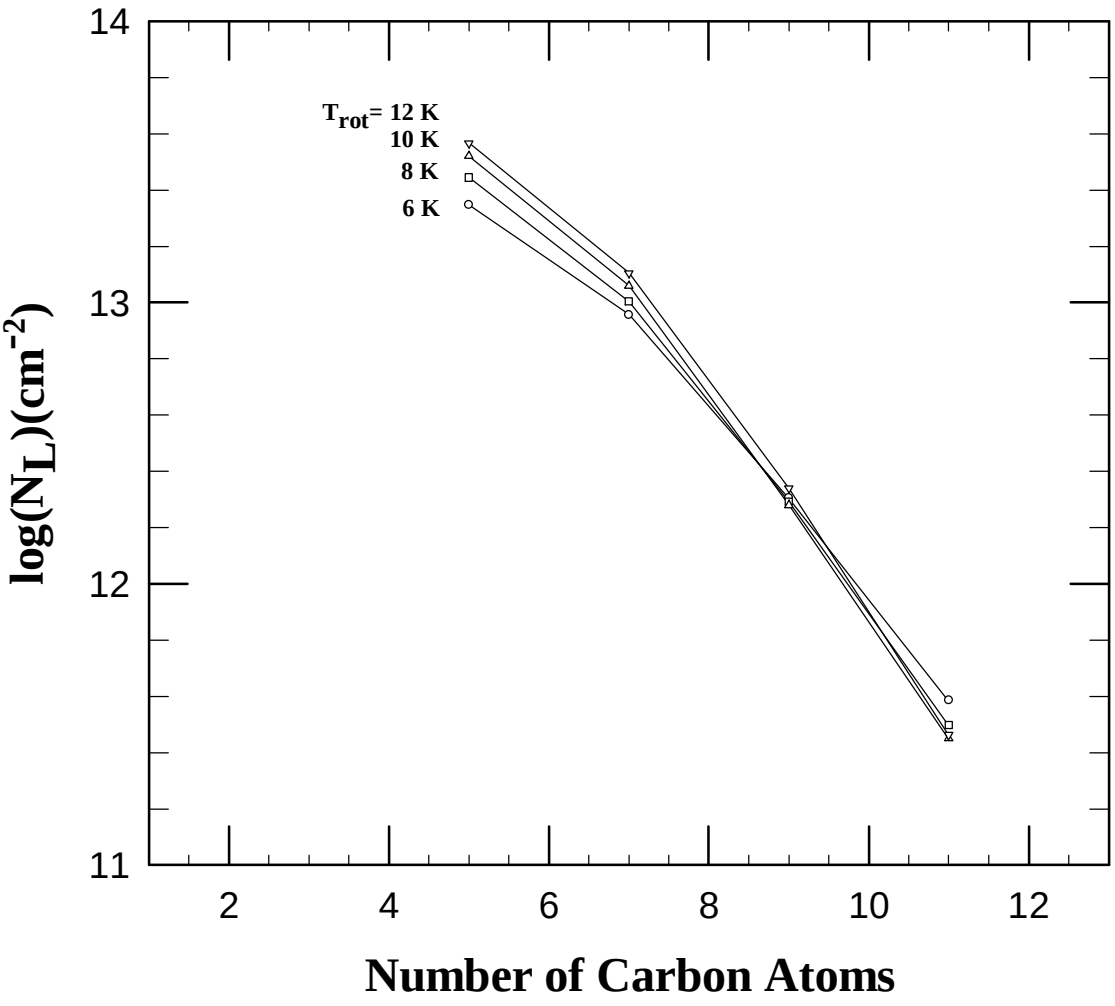
Fig. 1.— Spectra in TMC-1 of two lines of $HC_{11}N$ above one of HC_9N. Obtained by small-offset frequency switching, the spectra have been overlapped and the frequency-switched images removed.

Fig. 2.— Spectra (upper) of the $J = 5 \rightarrow 4$ transition of HC_5N, showing partially resolved quadrupole hyperfine structure, and (lower) of the $12 \rightarrow 11$ transition of HC_7N. The frequency-switched images have not been removed.

Fig. 3.— (top) Plot of the logarithm of the calculated column densities of the cyanopolyynes in TMC-1 from HC_5N to $HC_{11}N$ for the indicated excitation temperatures.(bottom) Plot of the decrements between successive odd-numbered cyanopolyynes in TMC-1 for the indicated excitation temperatures.


U13186.9
HC11N(J=39-38)
U13186.5
HC11N(J=38-37)
U12848.4
HC9N (J=23-22)
TA* (mK)
LSR Velocity (km s-1)


0.4
0.2
0.0
-0.2
T_A^*(K)
13313.0
13313.2
13313.4
13313.6
0.2
0.0
T_A^*(K)
13535.6
13535.8
13536.0
13536.2
13536.4
Frequency (MHz)


14
13
12
11
2
4
6
8
10
12
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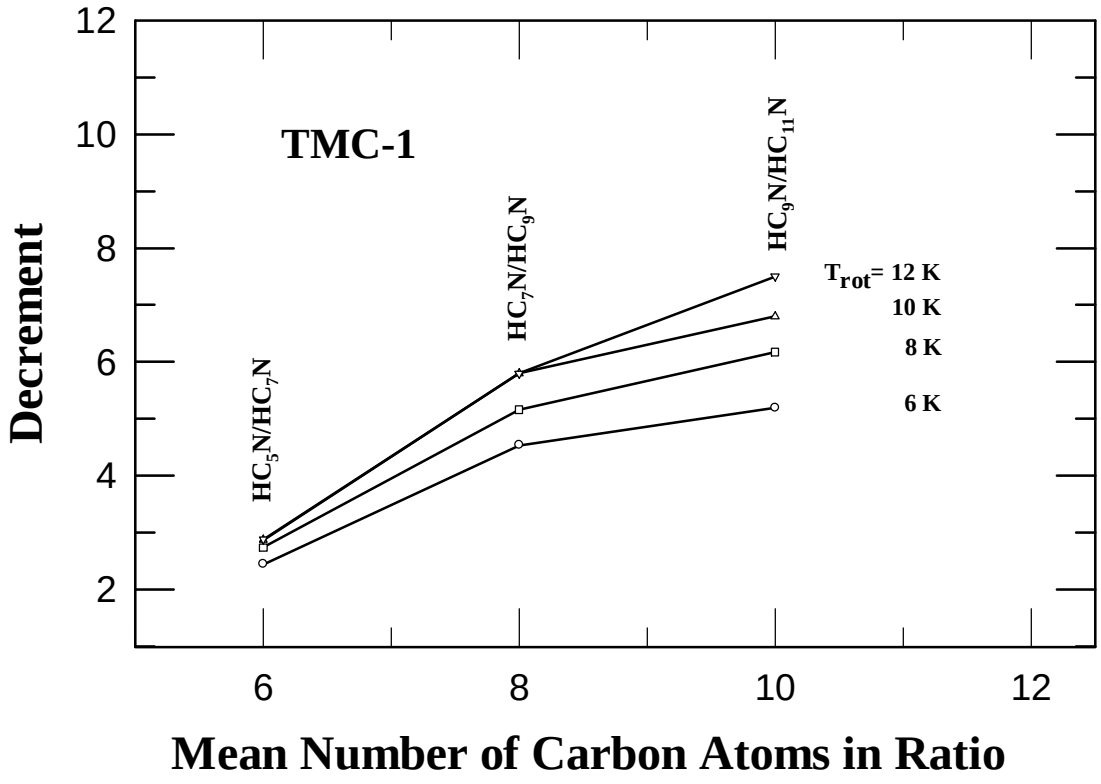
10 K
8 K
6 K
log(N_L)(cm^{-2})
Number of Carbon Atoms


12
10
8
6
4
2
6
8
10
12
TMC-1
HC_5N/HC_7N
HC_7N/HC_9N
$HC_9N/HC_{11}N$
T_{rot}= 12 K
10 K
8 K
6 K
Decrement
Mean Number of Carbon Atoms in Ratio